Non-Central Potentials and Spherical Harmonics Using Supersymmetry and Shape Invariance

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Abstract

It is shown that the operator methods of supersymmetric quantum mechanics and the concept of shape invariance can profitably be used to derive properties of spherical harmonics in a simple way. The same operator techniques can also be applied to several problems with non-central vector and scalar potentials. As examples, we analyze the bound state spectra of an electron in a Coulomb plus an Aharonov-Bohm field and/or in the magnetic field of a Dirac monopole.

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Spherical harmonics are introduced in physics courses while treating the Laplacian in spherical polar coordinates. In the context of quantum mechanics, the Schrödinger equation is separable into radial and angular parts if the potential is spherically symmetric. The angular piece of the Laplacian operator generates spherical harmonics which obey interesting and useful recursive formulae. With the advent of supersymmetric quantum mechanics (SUSYQM)[1-3] and the idea of shape invariance[4], study of potential problems in nonrelativistic quantum theory has received renewed interest. SUSYQM allows one to determine eigenstates of known analytically solvable potentials using algebraic operator formalism[5] without ever having to solve the Schrödinger differential equation by standard series method. However, the operator method has so far been applied only to one dimensional and spherically symmetric three dimensional problems.

The study of exact solutions of the Schrödinger equation with a vector potential and a non-central scalar potential is of considerable interest. In recent years, numerous studies[6-10] have been made in analyzing the bound states of an electron in a Coulomb field with simultaneous presence of Aharonov-Bohm (AB)[11] field and/or a magnetic Dirac monopole[12]. In most of these studies, the eigenvalues and eigenfunctions are obtained via separation of variables in spherical or other orthogonal curvilinear coordinate systems. The purpose of this paper is to illustrate that the idea of supersymmetry and shape invariance can be used to obtain exact solutions of such non-central but separable potentials in an algebraic fashion. In this method, it emerges that the angular part (as well as the radial part) of the Laplacian of the Schrödinger equation can indeed be dealt with using the idea of shape invariance. This is a novel method of generating interesting recurrence properties of spherical harmonics. In standard text books on quantum mechanics[13], properties of spherical harmonics are discussed from a different point of view. In this regard our approach is new and instructive in the sense that the radial and the angular pieces of the Schrödinger equation can both be treated within the same framework. The present work also gives insight into the solvability of certain three-dimensional problems. Basically, this is a consequence of both separability of variables and the shape invariance of the resulting one-dimensional problems.

The Schrödinger equation for a particle of charge e in the presence of a scalar potential $V(r,\theta,\phi)$ and a vector potential $\vec{A}(r,\theta,\phi)$ is (in units of $\hbar = 2m = 1$)

$$[\{-i\vec{\nabla} - e\vec{A}(r,\theta,\phi)\}^2 + V(r,\theta,\phi)]\psi = E\psi \quad . \tag{1}$$

We will consider vector potentials of the form $\vec{A} = \frac{F(\theta)}{r\sin\theta}\hat{e}_\phi$, and scalar potentials of the form $V = V_1(r) + \frac{V_2(\theta)}{r^2}$. The Schrödinger equation reads

$$\begin{aligned} -\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) - \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) - \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} & \\ + \left(\frac{e^2F^2(\theta)}{r^2\sin^2\theta} + V_1(r) + \frac{V_2(\theta)}{r^2}\right)\psi + \frac{2ieF(\theta)}{r^2\sin^2\theta}\frac{\partial\psi}{\partial\phi} &= E\psi. \end{aligned} \tag{2}$$

Eq. (2) permits a solution via separation of variables, if one writes the wave function in the form

$$\psi(r,\theta,\phi) = R(r)P(\theta)e^{im\phi} \quad . \tag{3}$$

The equations satisfied by the quantities $R(r)$ and $P(\theta)$ are:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(E - V_1(r) - \frac{l(l+1)}{r^2}\right)R = 0 \quad , \tag{4}$$

$$\frac{d^2P}{d\theta^2} + \cot\theta\frac{dP}{d\theta} + \left[l(l+1) - \frac{\{m - F(\theta)\}^2}{\sin^2\theta} - V_2(\theta)\right]P = 0. \tag{5}$$

Solutions of these equations for various choices of scalar and vector potentials will now be discussed.

Spherical Harmonics: Let us begin with the simplest case of a free particle [$V_1(r) = V_2(\theta) = F(\theta) = 0$.] This will allow us to obtain the standard properties of the spherical harmonics. In this case, differential equation (5) reduces to

$$\frac{d^2P}{d\theta^2} + \cot\theta\frac{dP}{d\theta} + \left[l(l+1) - \frac{m^2}{\sin^2\theta}\right]P = 0 \quad , \tag{6}$$

which is the equation satisfied by associated Legendre polynomials. To solve it by the SUSYQM method, we need to re-cast it into a Schrödinger-like equation. Changing the variable $\theta \to z$ through a mapping function $\theta = f(z)$, one obtains

$$\frac{d^2P}{dz^2} + \left[-\frac{f''}{f'} + f'\cot f\right]\frac{dP}{dz} + f'^2\left[l(l+1) - \frac{m^2}{\sin^2 f}\right]P = 0 \ . \tag{7}$$

Since we want the first derivative to vanish, we choose

$$\frac{f''}{f'} = f' \cot f \quad , \tag{8}$$

which gives

$$\theta \equiv f = 2 \tan^{-1}(e^z) \quad . \tag{9}$$

This transformation amounts to the replacement $\sin\theta = \mathrm{sech} z$ and $\cos\theta = -\tanh z$. The range of the variable z is $-\infty < z < \infty$. Eq. (6) now reads

$$-\frac{d^2 P}{dz^2} - l(l+1)\mathrm{sech}^2 z \; P = -m^2 \; P \quad . \tag{10}$$

This is a well-known, shape invariant, exactly solvable potential. It can be readily solved by standard SUSYQM techniques [3, 5]. The energy eigenvalues for the potential $V(z) = -a_0(a_0+1)\mathrm{sech}^2 z \;\; (a_0 > 0)$ are:

$$E_n = -(a_0 - n)^2 \quad ; \quad (n = 0, 1, 2, \cdots N) \quad , \tag{11}$$

where N is the number of bound states this potential holds, and is equal to the largest integer contained in a_0. The eigenfunctions $\psi_n(z, a_0)$ are obtained by using supersymmetry operators[5]:

$$\psi_n(z; a_0) \propto A^\dagger(z; a_0) A^\dagger(z; a_1) \cdots A^\dagger(z; a_{n-1}) \psi_0(z; a_n) \quad , \tag{12}$$

where $A^\dagger(z; a) \equiv \left(-\frac{d}{dz} + a \tanh z\right)$ and $a_n = a_0 - n$. The ground state wave function is $\psi_0(z; a_n) = \mathrm{sech}^{a_n} z$.

For our problem, $a_0 = l$, $E_n = -m^2$ and consequently one has

$$n = l - m \; ; \qquad P_{l,m}(\tanh z) \sim \psi_{l-m}(z; l), \tag{13}$$

where $P_{l,m}(\tanh z)$, the solutions of eq. (6), are the associated Legendre polynomials of degree l. Now that these $P_{l,m}(z)$ functions can be viewed as solutions of a Schrödinger equation, we can apply all the machinery one uses for a quantum mechanical problem. For example, we know that the parity of the n-th eigenfunction of a symmetric potential is given by $(-1)^n$, we readily deduce the parity of $P_{l,m}$ to be $(-1)^{l-m} = (-1)^{l+m}$[15]. Also, the application of supersymmetry algebra results in identities that are either not very well known or not easily available. With repeated application of the $A^\dagger$ operators, we can

determine $P_{l,m}$ for a fixed value $(l-m)$. As an illustration, we explicitly work out all the polynomials for $l-m=2$. The lowest polynomial corresponds to $l=2, m=0$. For a general l, using eq. (12), one gets

$$
\begin{aligned}
P_{l,l-2}(\tanh z) &\sim \psi_2(z;l) \\
&\sim A^\dagger(z;l)A^\dagger(z;l-1)\psi_0(z;l-2) \\
&\sim \left(-\frac{d}{dz}+l\tanh z\right)\left(-\frac{d}{dz}+(l-1)\tanh z\right)\operatorname{sech}^{l-2}z \\
&\sim \left[-1+(2l-1)\tanh^2 z\right]\operatorname{sech}^{l-2}z \quad .
\end{aligned} \tag{14}
$$

A similar procedure is readily applicable for other values of n. When one converts back to the original variable θ $(\operatorname{sech} z=\sin\theta\ ;\tanh z=-\cos\theta)$, the results are:

$$
\begin{aligned}
P_{l,l}(\cos\theta) &\sim \sin^l\theta \qquad (15)\\
P_{l,l-1}(\cos\theta) &\sim \sin^{l-1}\theta\cos\theta \\
P_{l,l-2}(\cos\theta) &\sim \left[-1+(2l-1)\cos^2\theta\right]\sin^{l-2}\theta \\
P_{l,l-3}(\cos\theta) &\sim \left[-3+(2l-1)\cos^2\theta\right]\sin^{l-3}\theta\cos\theta \\
P_{l,l-4}(\cos\theta) &\sim \left[3-6(2l-3)\cos^2\theta+(2l-3)(2l-1)\cos^4\theta\right]\sin^{l-4}\theta \\
P_{l,l-5}(\cos\theta) &\sim \left[15-10(2l-3)\cos^2\theta+(2l-3)(2l-1)\cos^4\theta\right]\sin^{l-5}\theta\cos\theta .
\end{aligned}
$$

These results are not readily available in standard books, although of course they can be obtained from the generating function for associated Legendre polynomials. Likewise, there are several recurrence relations which are easily obtainable via SUSYQM methods. In particular, by applying A or $A\dagger$ once, we generate recurrence relations of varying degrees (differ in l):

$$
\begin{aligned}
\psi_{l-m}(z,l)=A^\dagger(z,l)\psi_{l-m-1}(z,l-1) \;&\Longrightarrow\; P_{l,m}(x)=\left((1-x^2)\frac{d}{dx}+l\,x\right)P_{l-1,m} \qquad (16)\\
\psi_{l-m}(z,l)=A(z,l-1)\psi_{l-m+1}(z,l+1) \;&\Longrightarrow\; P_{l,m}(x)=\left((1-x^2)\frac{d}{dx}+(l-1)\,x\right)P_{l+1,m}.
\end{aligned}
$$

Non-Zero Vector Potential: Here we examine the general case with non-zero $F(\theta)$ in eq. (5). In particular, we consider

$$
F(\theta)=\frac{\mathcal{F}}{2\pi}+g(1-\cos\theta)\quad,\quad V_1(r)=-\frac{Ze^2}{r}\quad,\quad V_2(\theta)=0\quad . \tag{17}
$$

This choice corresponds to the physically interesting problem of the motion of an electron in a Coulomb field in the presence of an Aharonov-Bohm potential $\vec{A}_{AB} = \frac{\mathcal{F}}{2\pi r \sin\theta}\hat{e}_\phi$, and a Dirac monopole potential $\vec{A}_D = \frac{g(1-\cos\theta)}{r\sin\theta}\hat{e}_\phi$[10]. Both potentials can be chosen to be of arbitrary strength depending on the values of the coupling constants $\mathcal{F}$ and g. Again, we transform eq. (5) via the change of variables from θ to z given in eq. (9). The result is

$$\frac{d^2P}{dz^2} + [(\lambda^2 - \tilde{m}^2) - V(z)]P = 0 \quad , \tag{18}$$

with

$$V(z) = (\lambda^2 + q^2)\tanh^2 z - 2q\tilde{m}\tanh z \quad , \tag{19}$$

and

$$q = -ge \quad , \quad \tilde{m} = \frac{\mathcal{F}e}{2\pi} + ge - m \quad , \quad \lambda^2 = l(l+1) \quad . \tag{20}$$

The potential $V(z)$ has the form of the Rosen-Morse II potential, which is well-known to be shape invariant. More specifically, the potential

$$V_{RM}(z) = a_0(a_0+1)\tanh^2 z + 2b_0\tanh z \quad (b_0 < a_0^2) \tag{21}$$

has energy eigenvalues and eigenfunctions[5]

$$\begin{aligned} E_n &= a_0(a_0+1) - (a_0-n)^2 - \frac{b_0^2}{(a_0-n)^2}, \\ \psi_n &= (1-\tanh z)^{\frac{1}{2}\left[a_0-n+\frac{b_0}{a_0-n}\right]}(1+\tanh z)^{\frac{1}{2}\left[a_0-n-\frac{b_0}{a_0-n}\right]} P_n^{\left(a_0-n+\frac{b_0}{a_0-n},\, a_0-n-\frac{b_0}{a_0-n}\right)} . \end{aligned} \tag{22}$$

For our case, $E_n = \lambda^2 - \tilde{m}^2$ and the constants a_0, and b_0 are given by

$$a_0 = -\frac{1}{2} + \sqrt{\frac{1}{4} + (\lambda^2 + q^2)} \,, \qquad b_0 = -q\tilde{m} \quad .$$

Using these values and stipulating that eigenfunctions given in eq. (22) be normalizable, we get

$$\begin{aligned} n &= \sqrt{\tfrac{1}{4} + (\lambda^2 + q^2)} - |q| - \tfrac{1}{2} \qquad (|q| > |\tilde{m}|) \quad , \\ &= \sqrt{\tfrac{1}{4} + (\lambda^2 + q^2)} - |\tilde{m}| - \tfrac{1}{2} \qquad (|q| < |\tilde{m}|) \quad . \end{aligned} \tag{23}$$

Corresponding to these two cases, one gets

$$\begin{aligned} l &= -\tfrac{1}{2} + \sqrt{(n + |q| + \tfrac{1}{2})^2 - q^2} \qquad (|q| > |\tilde{m}|) \quad , \\ &= -\tfrac{1}{2} + \sqrt{(n + |\tilde{m}| + \tfrac{1}{2})^2 - q^2} \qquad (|q| < |\tilde{m}|) \quad . \end{aligned} \tag{24}$$

The energy eigenvalues obtained from eq. (4) for the Coulomb potential are

$$E_N = \frac{-Z^2 e^4}{4[N+l+1]^2} \quad . \tag{25}$$

Therefore, our final eigenvalues for a bound electron in a Coulomb potential as well a combination of Aharonov-Bohm and Dirac monopole vector potentials are

$$\begin{aligned} E_N &= \frac{-Z^2 e^4}{4\left[N+\frac{1}{2}+\sqrt{(n+|q|+\frac{1}{2})^2-q^2}\right]^2} \qquad (|q|>|\tilde{m}|) \quad , \\ &= \frac{-Z^2 e^4}{4\left[N+\frac{1}{2}+\sqrt{(n+|\tilde{m}|+\frac{1}{2})^2-q^2}\right]^2} \qquad (|q|<|\tilde{m}|) \quad , \end{aligned} \tag{26}$$

which agree with eqs. (32) and (33) respectively of ref. [10].

The above calculation using operator techniques in SUSYQM can also be carried out when the Coulomb potential is replaced by a harmonic oscillator. Potentials of this type have been studied by many authors using other approaches[9].

Non-Central Scalar Potential: As a final example, we consider the case of zero vector potential and a scalar piece consisting of the Coulomb potential and a non-central part $V_2(\theta)$. The angular piece satisfies a modified version of eq. (10):

$$\frac{d^2P}{dz^2} + \left[\mathrm{sech}^2 z\,\{l(l+1) - V_2(z)\} - m^2\right] \; P = 0 \quad . \tag{27}$$

This equation is the Schrödinger equation for one of the known shape invariant potentials provided the function $V_2(z)$ is chosen appropriately. The following three simple choices can be made: $V_2(z) = b\sinh z, b\sinh 2z, b\cosh^2 z$. These choices give rise to the Scarf II and Rosen-Morse II potentials[3] in eq. (27). In terms of θ, these choices correspond to non-central potentials with angular dependences $\cot\theta, \cot\theta\mathrm{cosec}\theta$ and $\mathrm{cosec}^2\theta$, respectively.

Here, we will treat the case $V_2(z) = b\sinh z$ in detail. The full potential in eq. (27) is $-l(l+1)\mathrm{sech}^2 z + b\mathrm{sech} z\tanh z$ and the role of energy is played by $-m^2$. Recall[3] that the potential $V(x) = (B^2 - A^2 - A)\mathrm{sech}^2 x + B(2A+1)\mathrm{sech} x \tanh x$ with $A > 0$ has eigenvalues $E_n = 2An - n^2 \;\; (n < A)$. In terms of our parameters, this implies

$$B(2A+1) = b \quad , \quad b^2 - A^2 - A = -l(l+1) \quad , \quad 2An - n^2 = -m^2 \quad . \tag{28}$$

Elimination of A, B leads to

$$l = -\frac{1}{2} + \sqrt{\frac{1}{4} + X} \tag{29}$$

with

$$X = \frac{(n^2 - m^2)}{2n} + \frac{(n^2 - m^2)^2}{4n^2} - \frac{n^2 b^2}{(n^2 - m^2 + n)^2} \quad . \tag{30}$$

Substitution for l into eq. (25) gives the eigenvalues for this problem. Although we have explicit energy eigenvalues and eigenfunctions, it is not clear whether the non-central potential we have considered has physical significance.

In conclusion, we mention that in this paper we have attempted to explore the effectiveness of the SUSYQM operator methods to obtain analytic solutions of Schrödinger systems in more than one dimensions. It is clear that the factorization technique which has so far been applied to only one dimensional or spherically symmetric three dimensional problems, can be equally useful for non-central separable problems for which one dimensional equations can be recast into Schrödinger equations with shape invariant potentials. Many interesting properties of spherical harmonics emerge naturally as a simple realization of this operator technique. One should also note that although, in this paper, we have focused on spherical polar coordinates, any orthogonal curvilinear coordinate system which is separable into Schrödinger-type equations with shape invariant potentials will allow similar algebraic analysis, and will have analytically solvable eigenvalues.

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